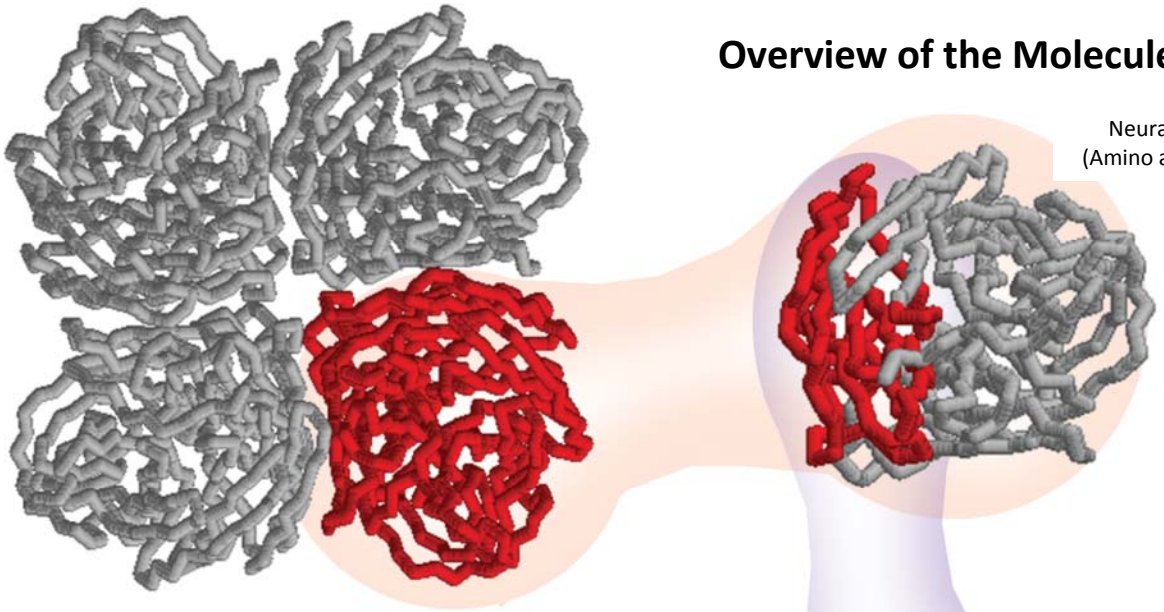
Guide to Using the Rubric to Score the Neuraminidase On-Site Model for Science Olympiad 2010 National Tournament

These instructions are to help the event supervisor and scoring judges use the rubric developed by the MSOE Center for BioMolecular Modeling when scoring the 2010 Science Olympiad **National Tournament On-Site Build** Mini-Toober models of influenza neuraminidase, based on **amino acids 116-235 of chain A from 2hu4.pdb**. Each category on the rubric is addressed within these instructions and is accompanied by a short description and picture, if appropriate.

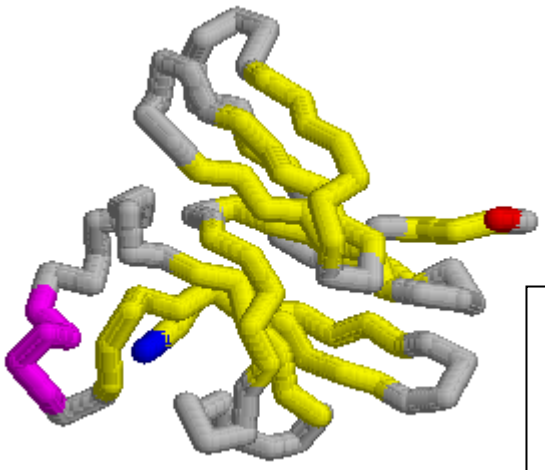
Overview of the Molecule:



Neuraminidase (4 chains)
Chain A in red

Neuraminidase Chain A
(Amino acids 116-235 in red)

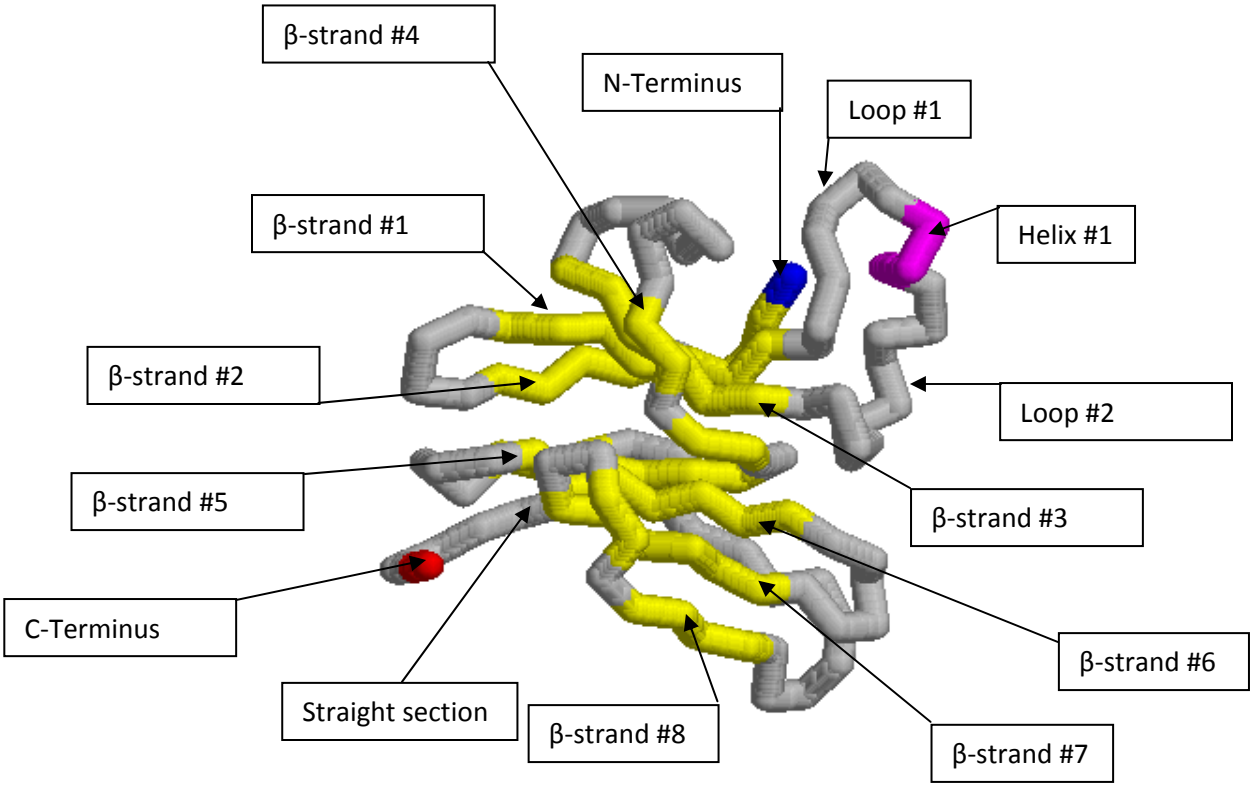
Neuraminidase Chain A
Amino acids 116-235



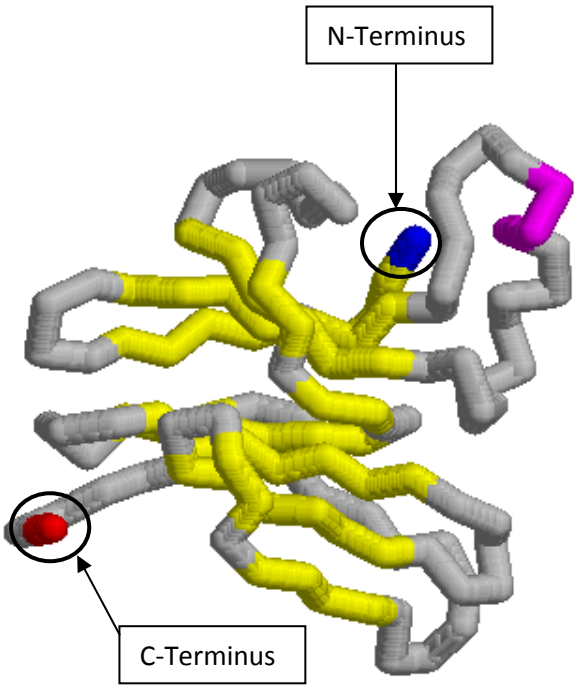
Color Code:
Yellow – beta strands
Magenta – helix
Gray – loops
Blue tip – N-terminus
Red tip – C-terminus

Order of Secondary Structures:

N-terminus → β-strand #1
Turn →β-strand #2
Loop #1 → α-helix #1
Loop #2 → β-strand #3
Loop #3 →β-strand #4
Turn→ β-strand #5
Turn →β-strand #6
Turn →β-strand #7
Turn →β-strand #8
Turn → Straight section/β-strand #9→C-terminus



1. Blue Cap on N-terminal Amino Acid (Val116) (1 pt)

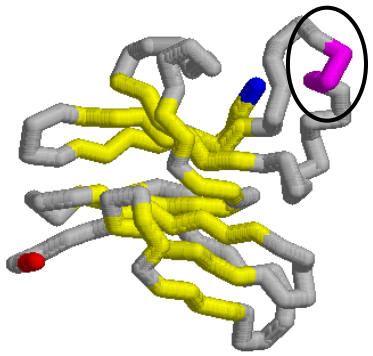


- To receive credit, the blue cap needs to be located at the N-terminus of the protein, which is located at the beginning of beta strand #1. Please see the figure to the right for the correct positioning of the blue end cap.
- The N-terminus is located closest to the helix.
- If the blue end cap is by the long straight region, then the model does not receive a point for this feature.

2. Red cap on C-terminal Amino Acid (Gly235) (1 pt)

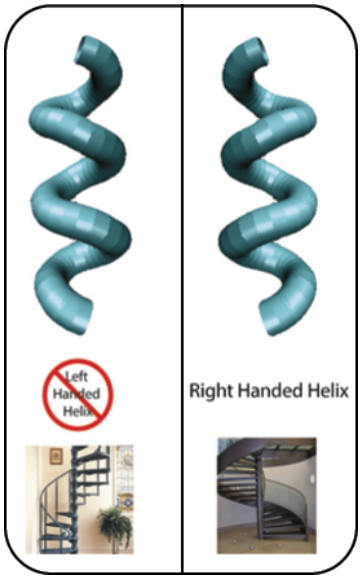
- To receive credit, the red cap needs to be located at the C-terminus of the protein, which is at the end of the long straight section. Please see the figure to the right for correct positioning of the red end cap.
- If the red cap is near beta strand #1 and close to the helix, then the model does not receive a point for this feature.

3. Model has 1 α-helix according to Jmol selection criteria (1 pt)



- To receive this point, there should be 1 helix within the model. Please see figure to the right for the correct location of this helix. (Helix is colored magenta on the model and on the figure to the right.)
- Deduct 0.5 point for each extra helix. For example, if a model has 2 helices, then the model would receive 0.5 pts rather than the full 1 point.

4. Alpha helices are right-handed (1 pt)



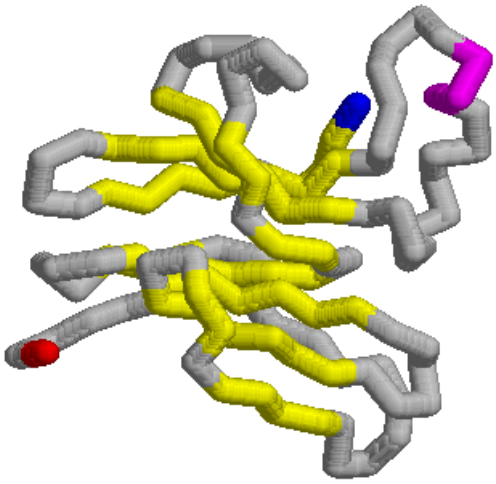
- Alpha helices are right-handed. Check each alpha helix in the model to confirm that the helix is right-handed. If the helix is right-handed, the model should receive 1 point.
- To determine if the helix is right-handed, find one of the ends of the helix and imagine that the helix is a spiral staircase. Imagine walking up the staircase with your hand on the handrail on the outside of the staircase. If your right hand is on the handrail as you climb up the staircase, you have a right-handed helix. If your left hand is on the handrail as you climb up the staircase, you have a left-handed helix and the modeled helix would not receive credit.
- Please refer to figure at left for illustration of left-handed and right-handed helices.

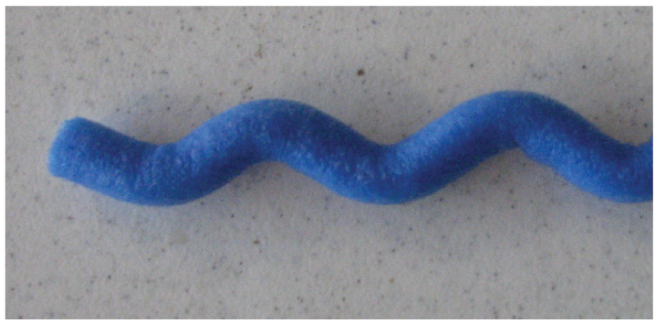
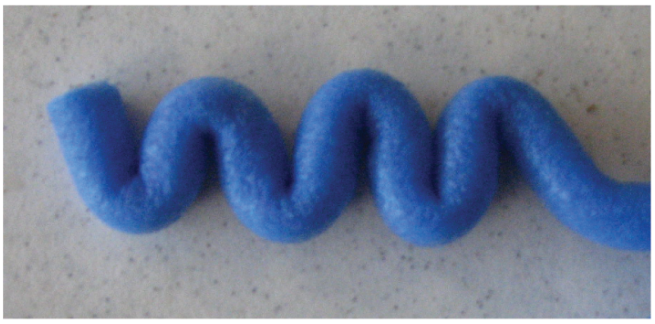
5. Alpha helix is the correct length. (0.5 pt)

- Helix #1 should have approximately 0.5-1.5 turns (3-5 amino acids in length).

6. Model has 9 β-strands according to Jmol selection criteria (0.5 pt per β-strand for a total of 4.5 points)

- To receive these points, there should be 9 β-strands within the model. Please see figure to the right for the correct location of these beta strands. (β-strands are colored yellow on the model and on the figure to the right.)
- β-strands need to be clearly distinguishable from loops; there may be some slight 'zig-zag' folding of the toober to indicate the up-and-down positioning of the amino acids. Alternately, teams might color-code their beta strands to distinguish them from loops or write on the toober indicating the location of the β-strands. Please see photos on the following page depicting β-strands.
- If there are more than 9 β-strands in this model, 0.5 pt should be deducted for each extra strand. For example, if the model has 10 β-strands, the model should receive 4 points, rather than the full 4.5 points.



	
This is a good example of a beta strand, slightly folded. It would also be acceptable to color code or in some other way mark the backbone to indicate beta sheets.	Although this model shows a beta strand, it is actually too kinked, such that the length of the beta strand is disproportionate to the width. If ALL of the beta strands are hyper-kinked, deduct 1 pt.

7. Positioning of secondary structures in proper order (0.5 pts each; for a total of 5 pts)

- To receive these points, the sequence of the secondary structures should be in the following order:

  N-terminus → β-strand #1
  Turn →β-strand #2
  Loop #1 → α-helix #1
  Loop #2 → β-strand #3
  Loop #3 →β-strand #4
  Turn→ β-strand #5
  Turn →β-strand #6
  Turn →β-strand #7
  Turn →β-strand #8
  Turn → Straight section/β-strand #9→C-terminus

- Please refer to the physical model or the illustrations on page 2 to help in visualizing the order of structures.

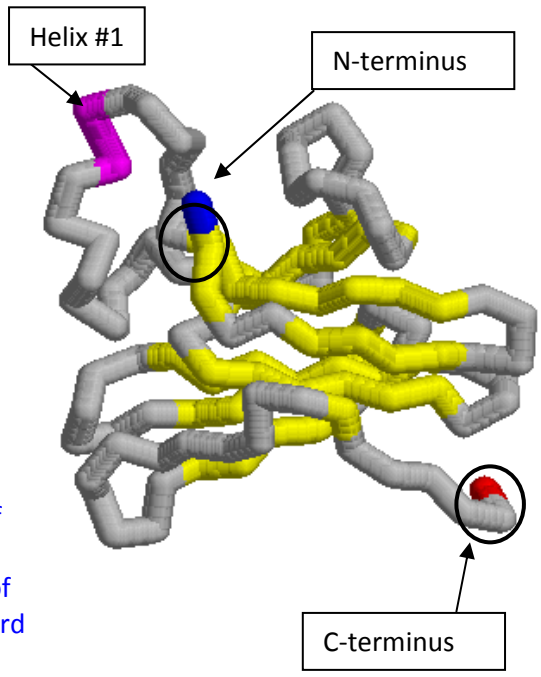
- Each bulleted sequence, if in the correct order, should receive 0.5 pt, for a total of 5 pts.

- Secondary structures that are out of order should not be counted.

Items #8-13 refer to the 3-dimensional shape of the model:

- The positioning of the secondary structures is very important to the overall 3-dimensional fold of the protein. Proteins are not flat; therefore the model should have a 3-dimensional look to it.

8. N and C termini are positioned correctly. (2 pts; 1 pt for being on the same "face" of the model and 1 pt for pointing in opposite directions on the same face)



- Hold the model so that the α-helix is on the top left and the N terminus is in the front of the model. Please refer to the picture on the right for correct orientation.

- In this orientation, the N and the C termini are on the same face of the protein (closest to you as you hold the model). Award 1 pt if the two termini are on the same face of the model. Note that the C terminus is in a strand that is at the front of the protein, but the C terminus is actually pointing back. If one terminus is located on the "back" of the model (farthest from you), deduct 0.5 pts.

- The N and C termini should be positioned on opposite sides of the same "face". The N-terminus is located on the "left side" (near helix) and the C-terminus is located on the "right side" of the model. If one of the termini is positioned incorrectly, award only 0.5 pt.

9. Model has 2 β-sheets (2 pts each for a total of 4 pts)

- This protein has two β-sheets arranged from the 9 β-strands. A β-sheet is composed of two or more β-strands lying parallel to each other, though the plane of the β-sheet may be twisted instead of flat.

- β-sheet #1 is composed of β-strands #1, #2, #3 and #4.

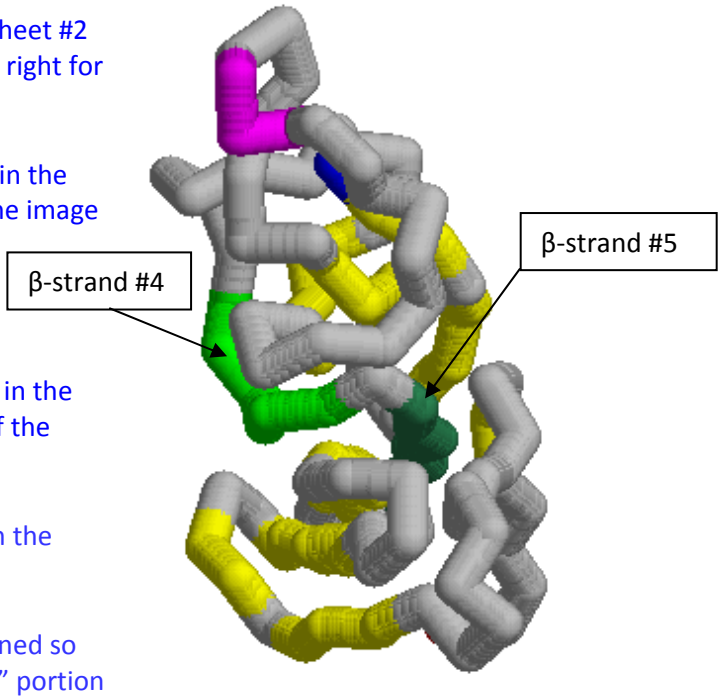
- β-sheet #2 is composed of β-strands #5, #6, #7, #8 and #9.

- To receive these points, β-strands 1-4 must be lying parallel to one another, forming one sheet. And β-strands 5-9 must be lying parallel to one another forming the second sheet.

- If the model has more than two β-sheets, then deduct 1 pt for each additional sheet. For example, if the model has three β-sheets, the model should receive 3 pts, rather than the full 4 pts.

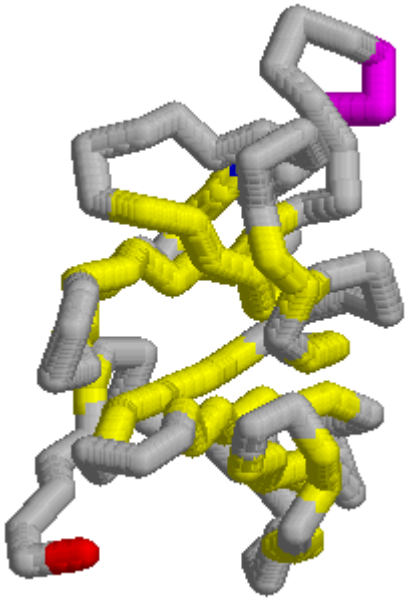
10. Orientation of β-strand #4 and β-strand #5 (2 pts)

- Hold the model so that the α-helix is on top and β-sheet #2 is on the bottom. Please refer to the picture on the right for correct orientation.
- β-strand #4 forms the last strand of β-sheet #1 and in the figure to the right, β-strand #4 is on the far left of the image and colored light green.
- β-strand #5 forms the first strand of β-sheet #2 and in the figure to the right, β-strand #4 is on the right side of the image and colored dark green.
- To receive 1 pt, β-strand #5 should be positioned on the opposite side of the model relative to β-strand #4.
- To receive 1 pt, the two β-strands should be positioned so that β-strand #4 is finishing the β-sheet on the "top" portion of the model and β-strand #5 is starting β-sheet #2 on the "bottom" portion of the model.

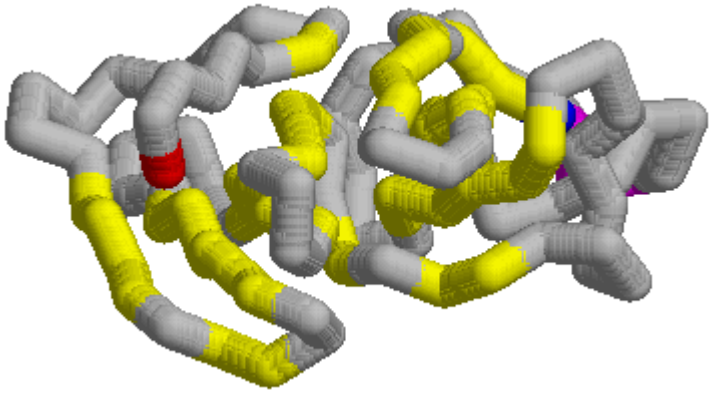


11. The two β-sheets in the model should be positioned so that the two β-sheets are on top of one another. (2 pts)

- Hold the model so that the C-terminus is located on the bottom left and the helix is located on the top right. Please refer to the picture on the right for correct orientation.
- β-sheet #1 should "sit" on top of β-sheet #2.
- The two sheets should overlap so that if you look "down the model", there should not be significant portions of the sheets extending beyond the central region of the model.
    - The sheets should not be positioned so that they are perpendicular to one another.
    - The sheets should not be positioned so that they are off-set from one another.

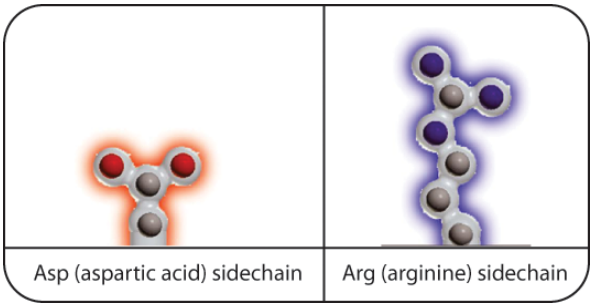


12. The model is compact. (2 pts)



- This is a compact protein, and therefore the model constructed by the team should reflect this compact structure.
- Award 2 pts if the model is compact.
- No points should be awarded if the model is constructed so that there is a lot of space between the sheets.

13. Correct positioning of the two amino acids Asp151 and Arg224 (4 pts)



- The provided amino acids should be positioned correctly within the sequence of the protein (Asp151 at position151, Arg224 at position 224). (1 pt for each sidechain correctly positioned at the right location in the protein.)
    - Asp151 is located immediately following helix #1 at the top of the loop.
    - Arg224 is located after the turn into the last straight section/β-strand #9.
- The amino acids should also be oriented correctly within 3-dimensional space. (1 pt for each sidechain correctly oriented)
    - Asp151 should be pointing toward the face of the model that has the N and C termini and out from the peak of the loop.
    - Arg224 should be pointing to the same side that Asp151 is pointing (the face with the N and C termini).
    - Both Asp151 and Arg224 should be located on the same side of the model (the left side, if holding the model as the image above is positioned). These two amino acids should lie in close proximity to each other. Please see figure to the right and the physical model for proper location and positioning.